(1,1'-Biphenyl)-2,2'-diol 1806-29-7 | DTXSID6051809

Model Performance

Model	Data

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 7.42

Global applicability domain: Inside

Local applicability domain index: 4.67e-01

Confidence level: 7.16e-01

Nearest Neighbors from the Training Set

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O,O-Diethyl dithiophosphate

Measured: 5.01 Predicted: 5.43

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2,2,4-Trimethyl-1,3-pentanediol

Measured: 1.00 Predicted: 1.47

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Dioxabenzofos Measured: 20.4 Predicted: 13.7

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2,2-Bis(bromomethyl)-1,3-

propanediol Measured: 4.79 Predicted: 3.35

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Methyl parathion Measured: 85.1 Predicted: 14.5